LA-UR-18-29476
Approved for public release; distribution is unlimited.

Title: Glassy dynamics in granular matter through flow heterogeneities: Shear-Transformation-Zone theory and applications in granular flow and nonlinear acoustics

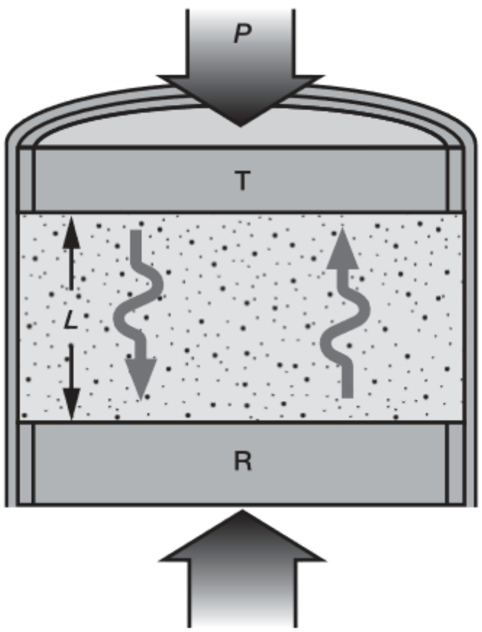
Author(s): Lieou, Charles Ka Cheong

Intended for: Invited talk at the ESPCI/Langevin Institute, Paris, Oct 16 2018

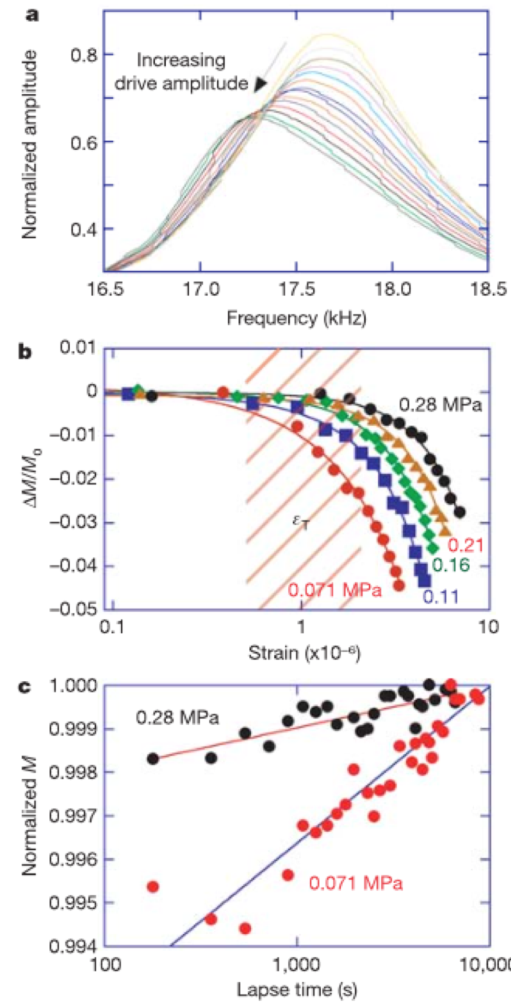
Issued: 2018-10-04

Glassy dynamics in granular matter through flow heterogeneities: Shear-Transformation-Zone theory and applications in granular flow and nonlinear acoustics

Charles Lieou
(with James Langer, Jean Carlson, Paul Johnson, and many others)
Theoretical Division
Los Alamos National Laboratory

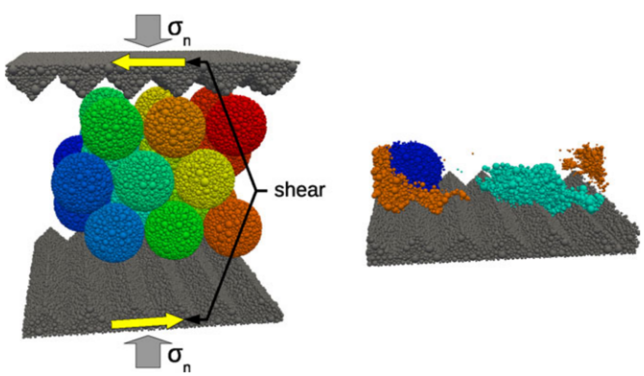


Oct 16 2018

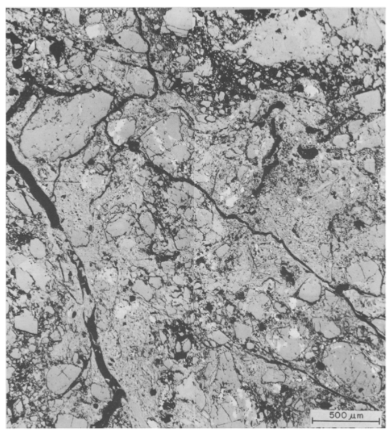


Flow in granular media

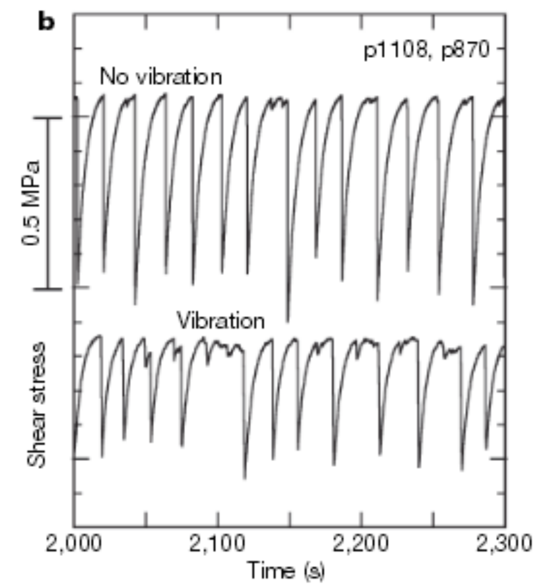
- Of relevance to materials processing, e.g., plastics, colloids, oil sand, tar sand, pharmaceuticals
- Natural phenomena, e.g., earthquakes, landslides, avalanches
- Strongly nonequilibrium phenomena of interest in physics



Mair and Abe (2011)

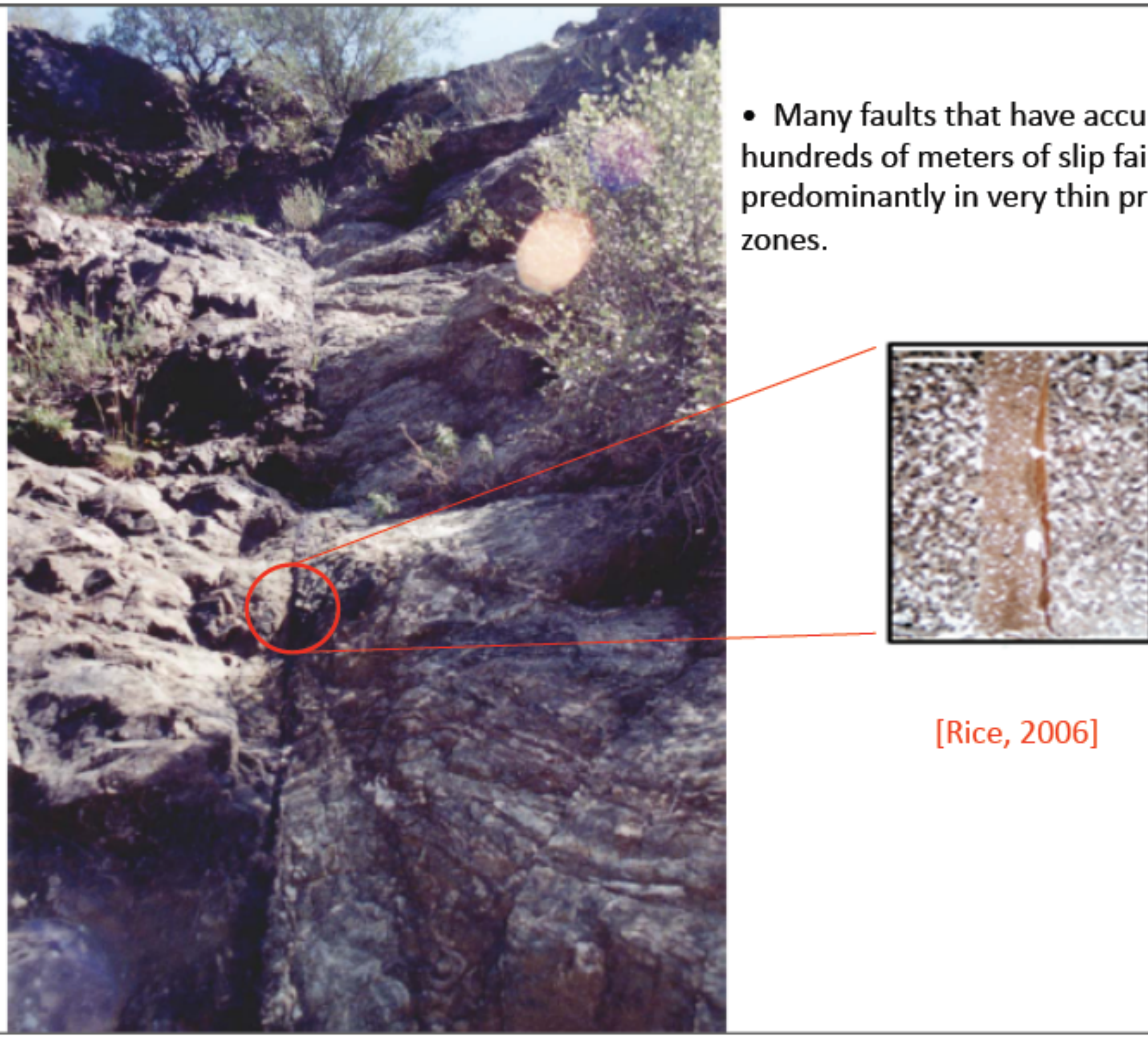


Sammis et al. (1987)



Johnson et al. (2008)

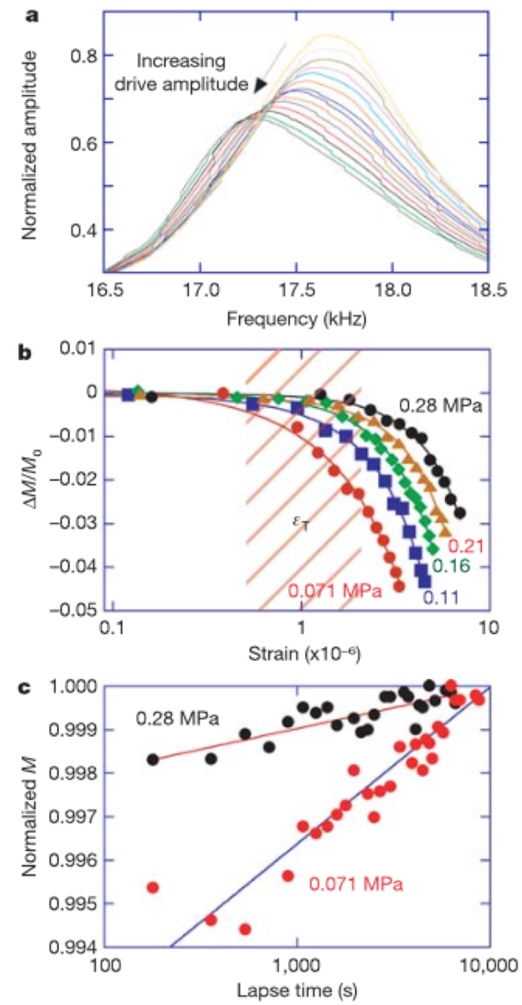
- Many faults that have accumulated hundreds of meters of slip fail predominantly in very thin primary slip zones.



[Rice, 2006]

Nonlinear behavior in glass bead packs

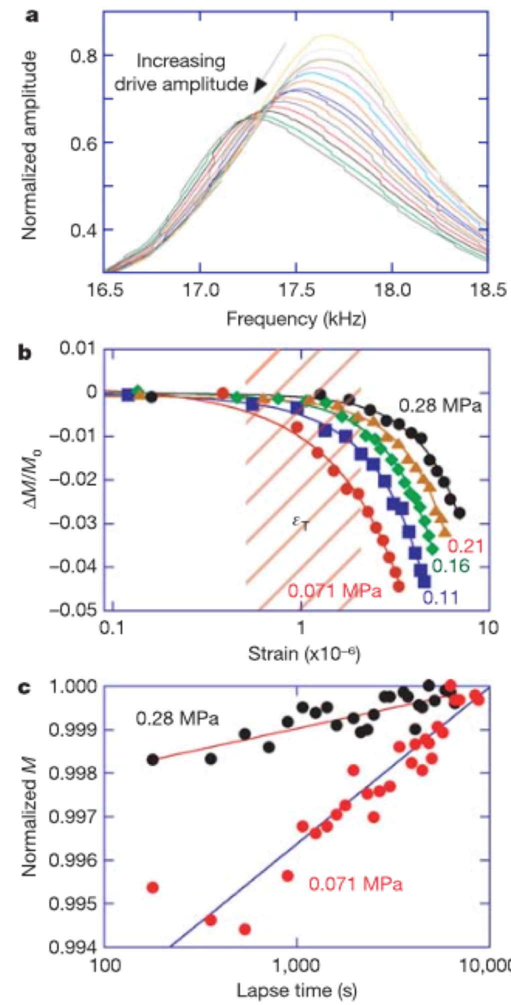
- ‘Fast nonlinear dynamics’ is evidenced by the change of the resonance frequency, and therefore the elastic moduli, as a function of the driving amplitude.
- ‘Slow dynamics’ seen with the gradual recovery of the elastic moduli upon cessation of acoustic vibration
- Similar behavior observed in consolidated granular materials
- In earth science, relevant to fault damage, wave velocity drop, and healing



P. A. Johnson and X. Jia, Nature (2005)

Nonlinear behavior in glass bead packs

- We focus on softening here.
- Slow relaxation of the granular glass bead pack after the cessation of external disturbances was addressed in CL et al., JGR (2017).
- We attribute deformation and plasticity to rearranging clusters of grains called shear transformation zones (STZs)
- Goal: to gain a unified understanding of the dynamics of driven granular media



P. A. Johnson and X. Jia, Nature (2005)

Outline

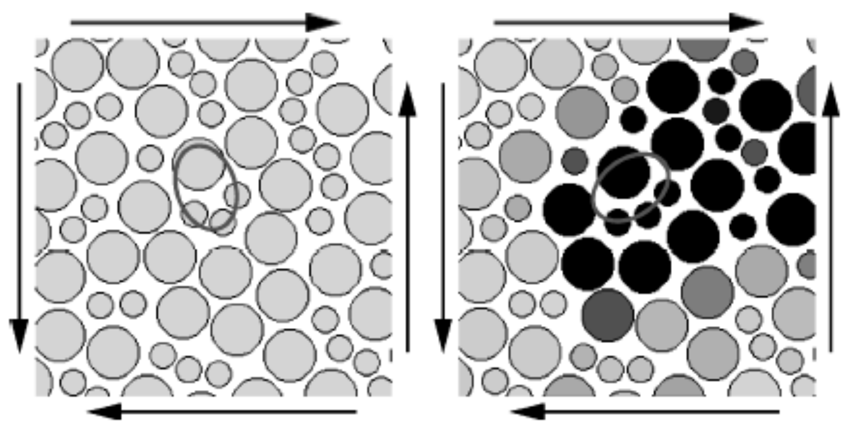
- STZ theory – an introduction
- Granular flow: stick-slip instabilities
- ‘Linearized’ STZ theory and wave perturbation
- Probing softening and resonance shift
- Glassy dynamics

Part I
STZ theory: an introduction

[C. K. C. Lieou and J.S. Langer, PRE 85, 061308 (2012)]

STZ's – microscopic description of shear deformation in granular media

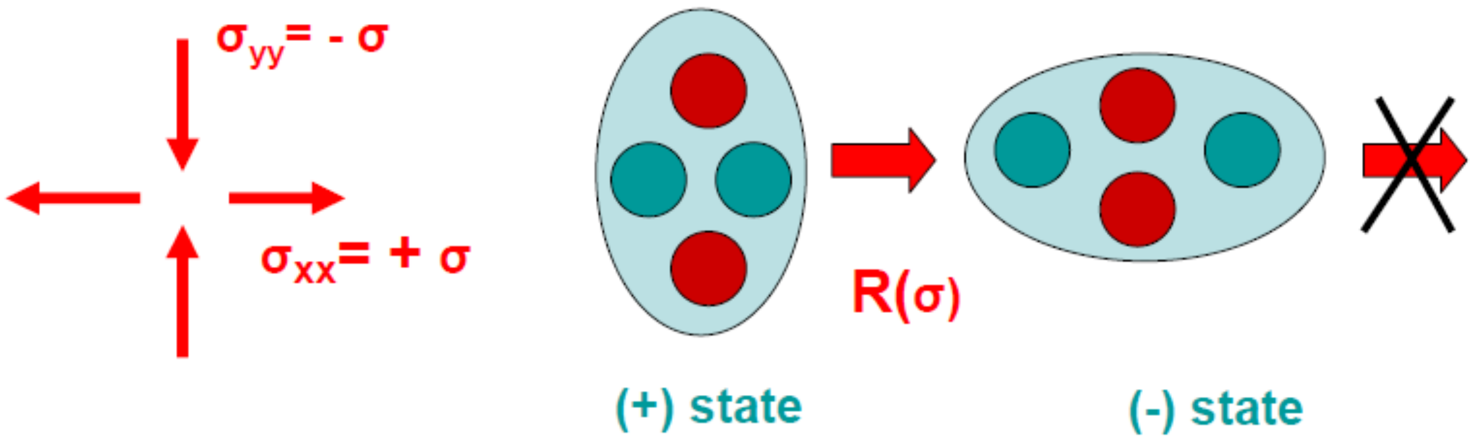
- Starting point: molecular/granular rearrangements lead to deformation of solids
- Shear transformation zones are local flow defects susceptible to shear deformation and contact change



[M. L. Falk and J. S. Langer, PRE 57, 7192 (1998)]

STZ theory: a short introduction

- To a good approximation, STZs come in two states; stable, and unstable, with respect to the deviatoric stress.



$$\boxed{\tau}\dot{N}_{\pm} = \boxed{\mathcal{R}(\pm\sigma)N_{\mp} - \mathcal{R}(\mp\sigma)N_{\pm}} + \boxed{\Gamma\left(Ne^{-1/\chi} - N_{\pm}\right)}$$

Molecular time scale (or inverse attempt frequency)

stress-driven transitions between the two possible states

noise-driven creation and annihilation of STZ defects

STZ theory: a short introduction

- The STZ density at the stationary state

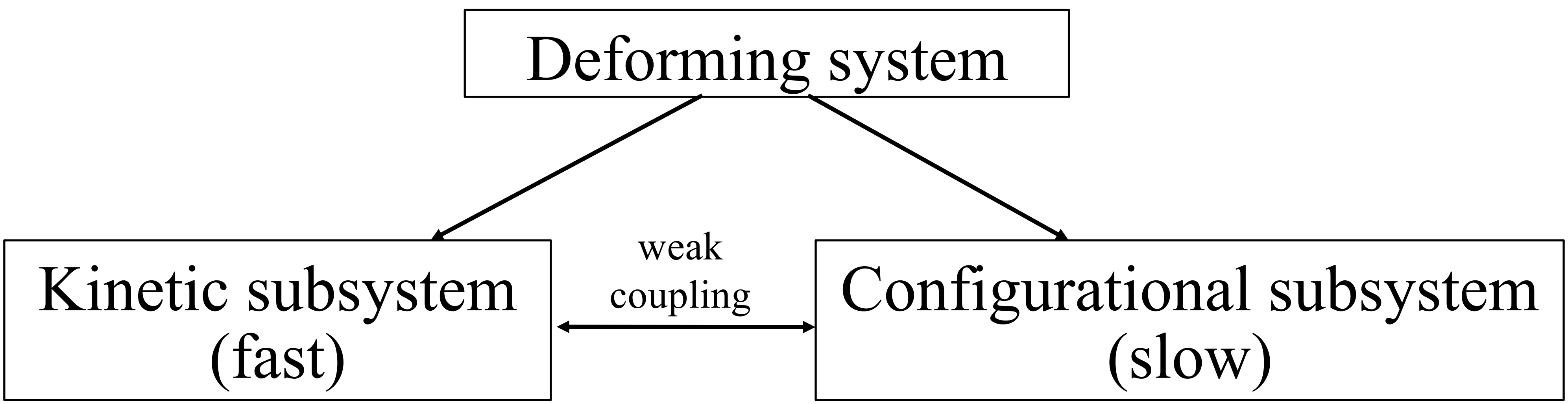
$$\Lambda \equiv \frac{N_+ + N_-}{N} = 2e^{-1/\chi}$$

is given by a thermodynamically-defined 'compactivity' with structural origins, reflecting disorder in the granular packing

- Let us briefly discuss the thermodynamic origins of the compactivity. Keep in mind: we want to describe the dynamics in a *statistical* fashion, without keeping track of every single grain.

Why thermodynamics?

- During the irreversible plastic deformation of a disordered solid, particle rearrangements drive the slow configurational degrees of freedom out of equilibrium with the heat bath.



Why thermodynamics?

- The kinetic-vibrational and configurational degrees of freedom are thus governed by two different temperatures – the "effective temperature" in the latter case.
- But in hard-spheres or particulate media, there is no intrinsic energy scale and no "configurational energy".

Why thermodynamics?

- Instead, the compactivity
$$X = \frac{\partial V}{\partial S_C}$$
characterizes the state of configurational disorder of a granular medium, with configurational entropy S_C.
- Analogous to temperature – but (configurational) energy is now replaced by volume.
- It can be shown that the STZ density relaxes toward the value
$$\Lambda = 2\exp\left(-\frac{v_Z}{X}\right)$$
where v_Z is the excess volume per STZ. For convenience, we use the *dimensionless* compactivity $\chi = X / v_Z$.

STZ theory: a short introduction

- Recall: the STZ density at the stationary state

$$\Lambda \equiv \frac{N_+ + N_-}{N} = 2e^{-1/\chi}$$

- Plastic deformation and flow occurs when STZ's 'flip' from one state to another, i.e., nonaffine rearrangement of grains (in the sense of change in contacts)

$$\dot{\epsilon}^{\mathrm{pl}} = \frac{\epsilon_0}{\tau N} e^{-1/\chi} \left(\mathcal{R}(\sigma) N_- - \mathcal{R}(-\sigma) N_+\right)$$

STZ theory: a short introduction

- STZ orientational bias

$$m \equiv \frac{N_+ - N_-}{N_+ + N_-}$$

- Define combinations of rate factors

$$\mathcal{C}(\sigma) = \frac{\mathcal{R}(\sigma) + \mathcal{R}(-\sigma)}{2}; \quad \mathcal{T}(\sigma) = \frac{\mathcal{R}(\sigma) - \mathcal{R}(-\sigma)}{\mathcal{R}(\sigma) + \mathcal{R}(-\sigma)}$$

- After change of variables

$$\begin{aligned} \tau \dot{m} &= 2\mathcal{C}(\sigma)\left(\mathcal{T}(\sigma) - m\right)\left(1 - \frac{m\sigma}{\sigma_0}\right); \\ \tau \dot{\epsilon}^{\mathrm{pl}} &= 2\epsilon_0 e^{-1/\chi}\mathcal{C}(\sigma)\left(\mathcal{T}(\sigma) - m\right). \end{aligned}$$

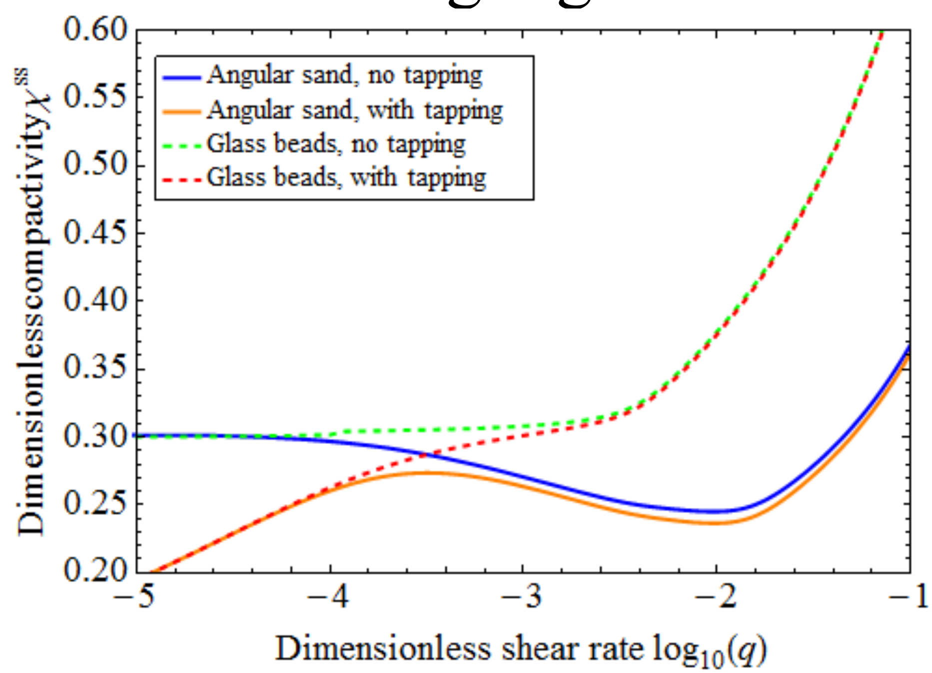
- It can be shown that $\mathcal{T}(\sigma) = \tanh[\epsilon_0\sigma/(\epsilon_Z\sigma_p\chi)]$ (σ_p = pressure)

Part II
Granular flow: stick-slip instabilities

[C. K. C. Lieou et al.,
Phys. Rev. E 92, 022209 (2015);
J. Geophys. Res. 121, 1483-1496 (2016);
J. Geophys. Res. 122, 295-307 (2017)]

Non-monotonicity implies instability?

- There is a one-to-one correspondence between the compactivity χ and the experimentally-measured layer thickness or volume. For frictional particles we observe non-monotonicity.
- If the minimum flow stress varies with χ in that region, then there can be a rate-weakening regime.



What controls the compactivity?

- The compactivity is controlled by the strain rate and the vibration intensity – again from experiments.
- It may make sense to consider the vibration-controlled compactivity and the shear-controlled compactivity on the same footing: both pertain to the configurational subsystem, especially if the underlying time scales are not too different.

$$\chi^{ss} = \hat{\chi}(q)$$

Shearing only, no vibrations or interparticle friction

$$\chi^{ss} = \tilde{\chi}(\rho)$$

Unsheared, vibrations only

What controls the compactivity?

- Also, for strongly vibrated granular media, the (irreversible) work done by vibrations may not be negligible – may need to properly take this into account.

$$\epsilon_1 \dot{\chi} = \mu \dot{\gamma}^{\text{pl}} + \boxed{\frac{Y}{\tau}} - \boxed{\mathcal{K}(\chi)}\chi.$$

work done by external acoustic vibrations

coupling to the environment (thermal temperature $T = 0$)

$$\mathcal{K}(\chi) = \frac{1}{\tau}\left[\frac{\boxed{W} + \boxed{F}}{\hat{\chi}(q)} + r\frac{\boxed{Y}}{\tilde{\chi}(\rho)}\right]$$

shearing

interparticle friction

vibrations

$$r \equiv \exp(-q^2/\rho)$$

Shear rate sets up a time scale above which vibrations cannot compete with shearing to cause grains to explore configurations – exponential cut-off

What controls the compactivity?

- Dynamical equations:

$$\dot{\mu} = (G/p)\boxed{(\dot{\gamma} - \dot{\gamma}^{\mathrm{pl}})},$$

Assume linear elasticity; elastic strain rate is difference between total and plastic parts

$$\begin{aligned} \dot{\chi} \;&=\; \frac{2\epsilon_0\mu_0 e^{-1/\chi}}{\tau\epsilon_1}\left[\boxed{\Gamma\left(1 - \frac{\chi}{\hat{\chi}(q)}\right)} - \boxed{\xi\,\frac{\chi}{\hat{\chi}(q)}}\right] \\ &+ \boxed{\frac{A_0\rho}{\tau\epsilon_1}\left[1 - \exp\left(-\frac{q^2}{\rho}\right)\frac{\chi}{\tilde{\chi}(\rho)}\right]} \; . \end{aligned}$$

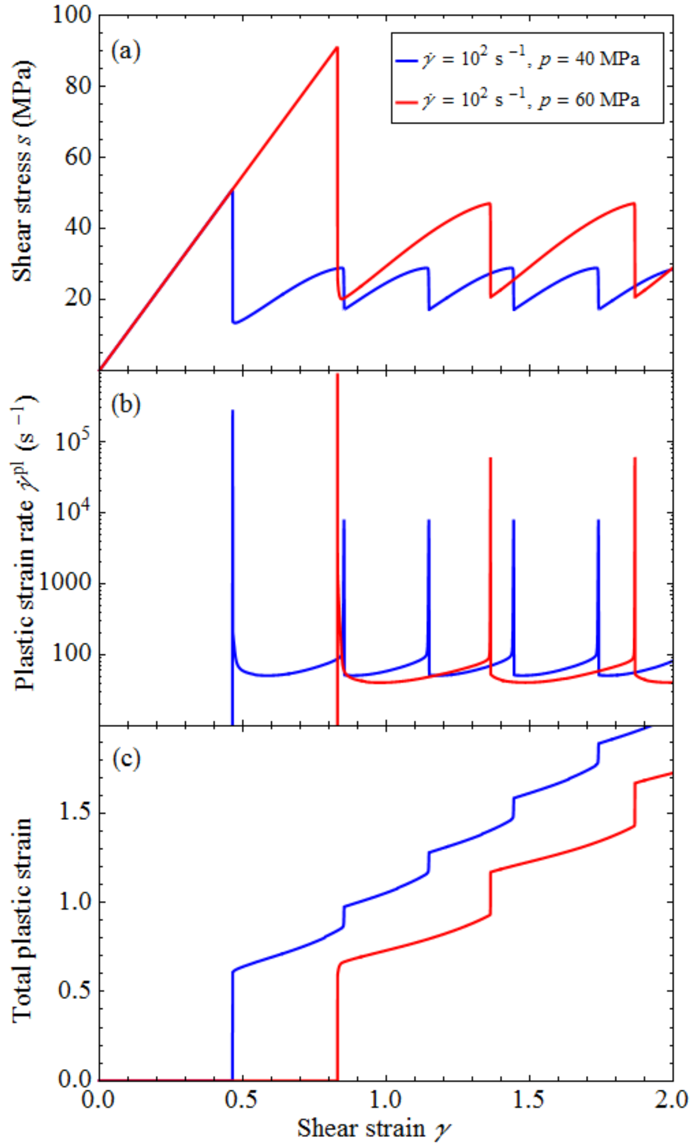
Shearing drives towards hard-sphere state

Friction generates internal acoustic noise

Vibrations compactify to some state determined by vibration intensity

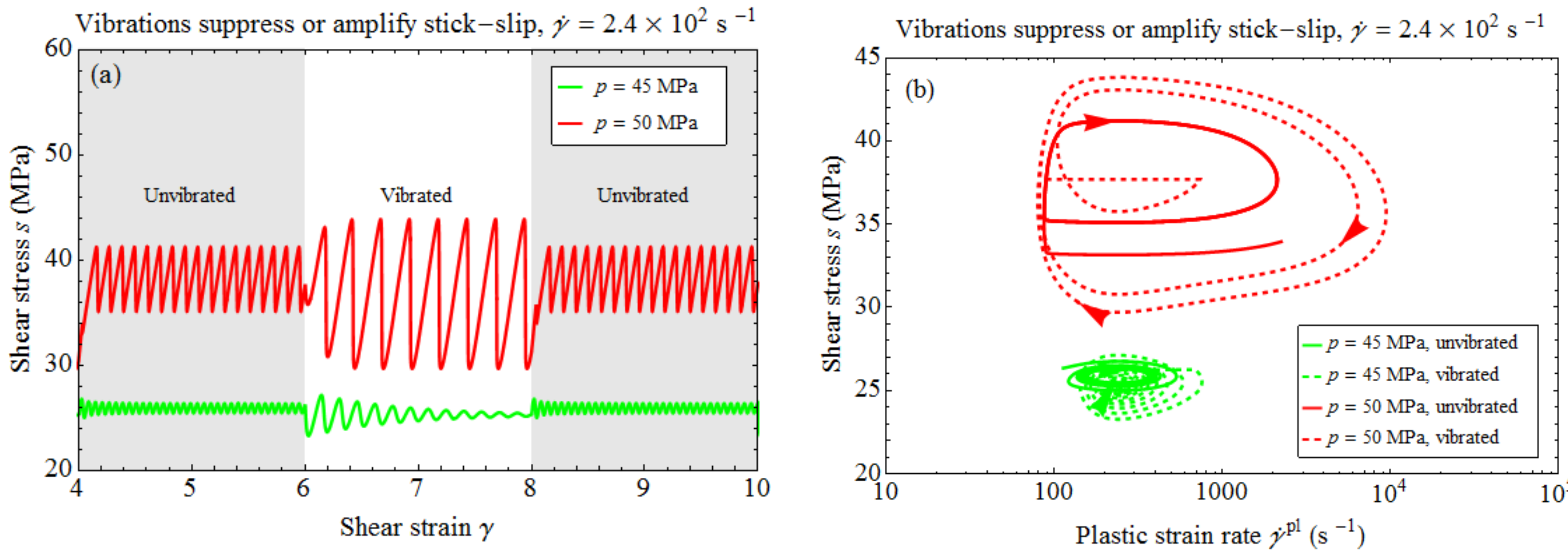
- The equation for χ is a consequence of the first law of thermodynamics.
- We show below that interparticle friction causes stick-slip instabilities.

Theoretical predictions



- Stick phase corresponds to small but nonzero plastic strain rate, giving rise to creep and rounding of stress-strain curve
- "Preseismic slip" in geophysical terms
- Slip phase corresponds to dramatic increase of plastic strain rate and large displacement

Theoretical predictions



- Vibrations control stick-slip – may amplify amplitude, or suppress stick-slip after transient
- Short transient upon switching on or off of vibrations

Part III
'Linearized' STZ theory and wave perturbation
[C. K. C. Lieou et al., J. Geophys. Res. 122(9), 6998-7008 (2017), and unpublished work]

Wave perturbation: linearize STZ equations

- Consider pressure waves for the time being; formulation for shear waves is almost identical
- Let σ be the stress amplitude
- Linearize STZ equations around the small quantities m and σ:

$$
\begin{aligned}
\tau \dot{m} &= 2R_0 \left(\frac{\Omega \sigma}{\chi} - m \right); \\
\tau \dot{\epsilon}^{\mathrm{pl}} &= 2R_0 \epsilon_0 e^{-1/\chi} \left(\frac{\Omega \sigma}{\chi} - m \right)
\end{aligned}
$$

Here $\Omega \equiv \epsilon_0/(\epsilon_Z \sigma_p)$

Wave perturbation: linearize STZ equations

- Combine these with the equations of motion:

$$\dot{\sigma} = \boxed{M_0}(\dot{\epsilon} - \dot{\epsilon}^{\mathrm{pl}}),$$

Unperturbed modulus at max. packing fraction

$$\rho_G \ddot{u} = \frac{\partial \sigma}{\partial x} + \boxed{F,} \qquad \boxed{\epsilon = \frac{\partial u}{\partial x}}$$

External forcing

Total strain in terms of displacement

- Use the ansatz

$$\begin{aligned} u &= \hat{u} e^{i(kx-\omega t)}; \\ \sigma &= \hat{\sigma} e^{i(kx-\omega t)}; \\ m &= \hat{m} e^{i(kx-\omega t)}; \\ F &= \hat{F} e^{i(kx-\omega t)}. \end{aligned}$$

Wave perturbation: linearize STZ equations

- The result is

$$
\begin{aligned}
-\omega^2 \rho_G \hat{u} &= ik\hat{\sigma} + \hat{F}; \\
-i\omega\hat{m} &= \alpha\left(\frac{\Omega\hat{\sigma}}{\chi} - \hat{m}\right); \\
-i\omega\hat{\sigma} &= M_0\left[k\omega\hat{u} - \alpha\epsilon_0 e^{-1/\chi}\left(\frac{\Omega\hat{\sigma}}{\chi} - \hat{m}\right)\right]
\end{aligned}
$$

where $\alpha \equiv 2R_0/\tau$.

- Eliminating *m* and *σ* gives

$$
\hat{F} = \rho_G \frac{(\omega_0^2\alpha - \omega^2\beta) - i\omega(\omega_0^2 - \omega^2)}{\beta - i\omega}\hat{u}
$$

with $\beta \equiv \alpha(1 + M_0\epsilon_0\Omega e^{-1/\chi}/\chi)$, and $v = \sqrt{\frac{M_0}{\rho_G}} = \frac{\omega_0}{k}$.

Part IV
Probing softening and resonance shift

Response function

- The relation between drive amplitude F (corresponding to, e.g, voltage) and response amplitude u

$$\hat{F} = \rho_G \frac{(\omega_0^2 \alpha - \omega^2 \beta) - i\omega(\omega_0^2 - \omega^2)}{\beta - i\omega} \hat{u}$$

prompts us to define the 'response function'

$$A(\omega) \equiv \frac{\beta - i\omega}{(\omega_0^2 \alpha - \omega^2 \beta) - i\omega(\omega_0^2 - \omega^2)}$$

- The norm of $A(\omega)$ gives the normalized strain amplitude; probing $A(\omega)$ gives the tuning curves and resonance peaks.

Modulus softening

- The ‘softened’ modulus M is given in terms of the resonance frequency ω_{res} and the system size H by

$$\omega_{\text{res}}^2 = \left(\frac{\pi}{H}\right)^2 \frac{M}{\rho_G}$$

- What controls the resonance frequency? Recall that

$$A(\omega) \equiv \frac{\beta - i\omega}{(\omega_0^2\alpha - \omega^2\beta) - i\omega(\omega_0^2 - \omega^2)}$$

$$\beta \equiv \alpha(1 + M_0\epsilon_0\Omega e^{-1/\chi}/\chi)$$

If the compactivity χ varies with the strain amplitude (reasonable), the resonance frequency may shift!

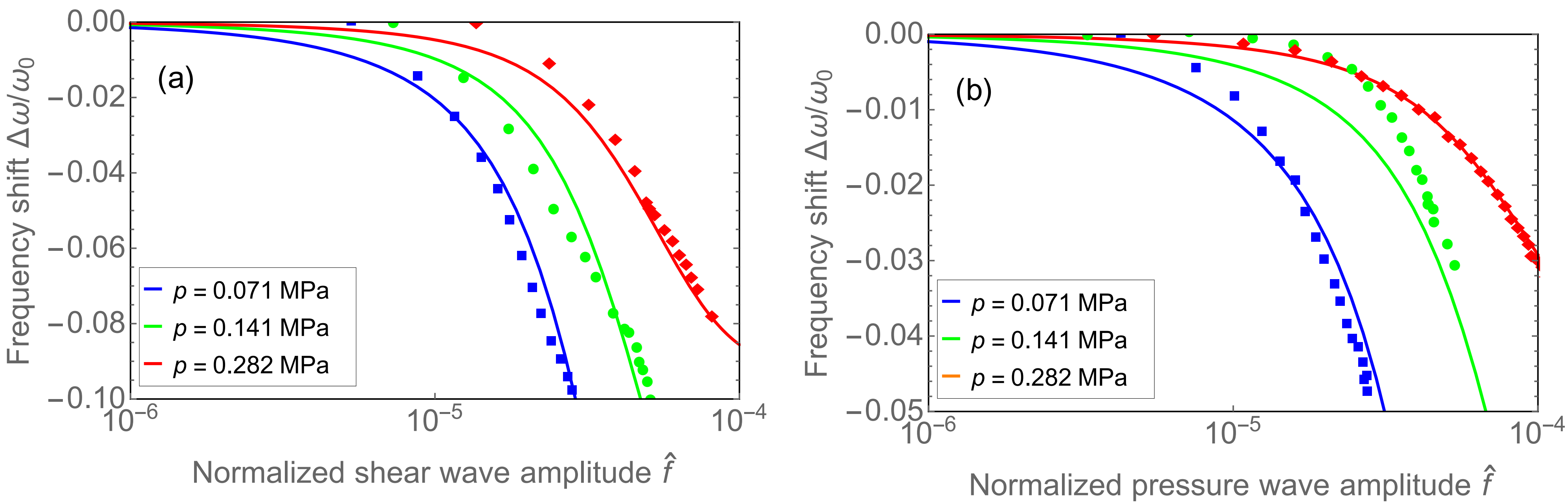
Modulus softening

- Intuition: the compactivity χ must be an increasing function of the strain amplitude.
- More strain => Higher compactivity => More STZ defects => Granular material becomes softer!
- To fit with the experimental softening data, use the ansatz

$$\chi(\hat{f}) = \chi_0 + \chi_1 \tanh(k_0 \boxed{\hat{f}})$$

Dynamic strain amplitude

Modulus softening

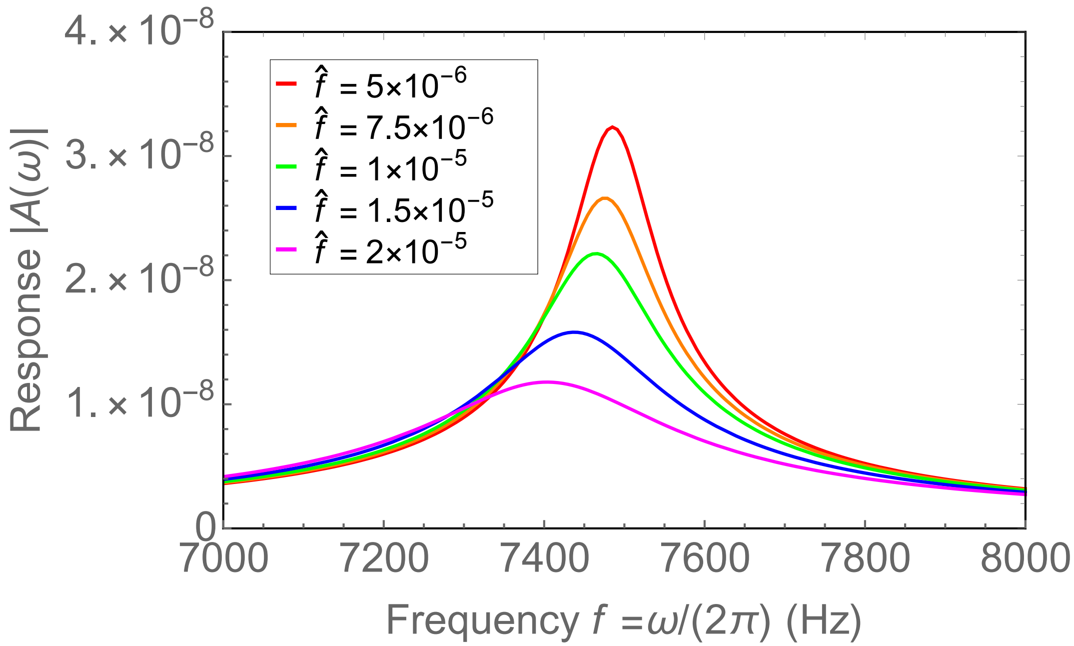


Resonance shift

- By directly computing the response function

$$A(\omega) \equiv \frac{\beta - i\omega}{(\omega_0^2\alpha - \omega^2\beta) - i\omega(\omega_0^2 - \omega^2)}$$

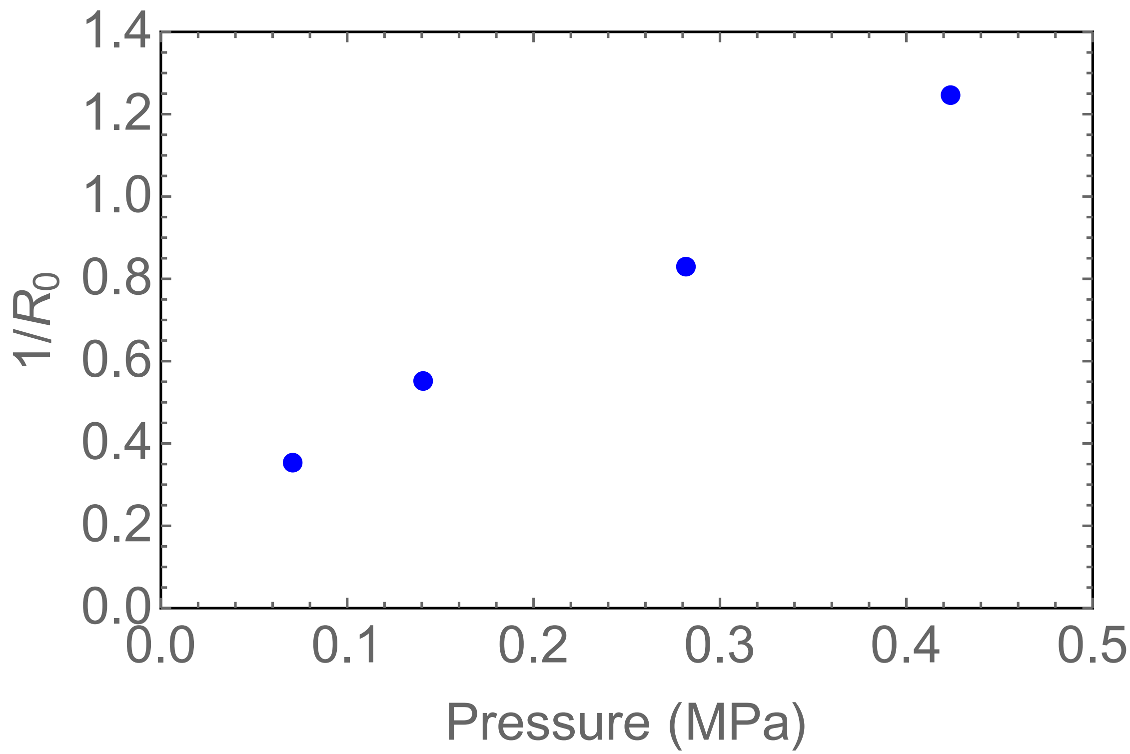
we can get the tuning curves (here shown for shear mode at $p = 0.282$ MPa):



Part V
Glassy dynamics

STZ event rate, measured by fitting

- The inverse STZ event rate $1/R_0$, or the STZ event rate itself, offers a deep probe of glassy dynamics in the weakly perturbed granular packing:



- Is this related to STZ size?

Probing connection between time scale and size distributions

- If one can trace and visualize the motion of grains, one could use the so-called $D^2{}_{\mathrm{min}}$ criterion

$$D^2_{\mathrm{min}}(i) \equiv \min_{\Lambda}\left\{\frac{1}{z}\sum_j [R_{ij}(t+\Delta t) - \Lambda R_{ij}(t)]^2\right\}$$

[Falk and Langer, PRE, 1998]

- Or the four-point correlation function [Abate and Durian, PRE, 2007]

$$Q_t(l,\tau) = \frac{1}{N}\sum_{i=1}^{N} w_i,$$

$$Q(l,\tau) = \langle Q_t(l,\tau)\rangle,$$

$$\chi_4(l,\tau) = N[\langle Q_t(l,\tau)^2\rangle - \langle Q_t(l,\tau)\rangle^2].$$

Probing connection between time scale and size distributions

- These measures tell us the heterogeneity of the particle displacements, and could tell us about the location of dynamical heterogeneities, aka STZs.
- Does the STZ size distribution bear any resemblance to the rate or time scale distribution? In the high-pressure regime where $1/R_0$ is large, do the STZs mostly appear in the form of large clusters of dynamical heterogeneities? If yes, this will be very interesting.

Concluding remarks

- STZ theory describes defect dynamics and plasticity in granular materials
- Addresses inadequacies in other empirical theories
- Compactivity – describing structural disorder – is key variable that controls defect density
- STZ theory describes granular flow and stick-slip.
- Coupling linearized STZ theory with wave equations generates modulus softening and downwards resonance shift with increasing strain amplitude
- Shows definitively that STZ defects are responsible for softening and dissipative, nonlinear behavior